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ME469: Common Discretization Approaches

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U.S. DEPARTMENT OF ENERGY

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Lecture Objectives

- The Concept of Meshing and Solving a Simple Model Equation
- Why Unstructured?
- Unstructured Element Types
- Cell-centered Finite Volume (FV)
- Edge-based Vertex-Centered (EBVC)
- Control-Volume Finite Element Method (CVFEM)
- Finite Element Method (FEM)
- Staggered arrangement

Recall, our Simple Model Equation

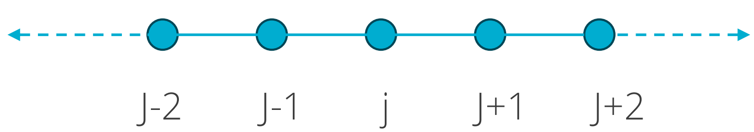
- With terms: time, advection and diffusion

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2}$$

- For a finite difference, centered (2nd order stencil), the continuous PDE can be discretized as:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}}{2\Delta x} = \nu \frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{\Delta x^2}$$

- Noting, above the n+1 fully implicit approach that is solved over the finite difference "mesh"



- What is an alternative? Finite-volume/element.....

Derivative	Accuracy	−5	−4	−3	−2	−1	0	1	2	3	4	5
1	2					−1/2	0	1/2				
	4				1/12	−2/3	0	2/3	−1/12			
	6			−1/60	3/20	−3/4	0	3/4	−3/20	1/60		
	8		1/280	−4/105	1/5	−4/5	0	4/5	−1/5	4/105	−1/280	
2	2					1	−2	1				
	4				−1/12	4/3	−5/2	4/3	−1/12			
	6			1/90	−3/20	3/2	−49/18	3/2	−3/20	1/90		
	8		−1/560	8/315	−1/5	8/5	−205/72	8/5	−1/5	8/315	−1/560	

Central finite difference

Derivative	Accuracy	0	1	2	3	4	5	6	7	8
1	1	−1	1							
	2	−3/2	2	−1/2						
	3	−11/6	3	−3/2	1/3					
	4	−25/12	4	−3	4/3	−1/4				
	5	−137/60	5	−5	10/3	−5/4	1/5			
	6	−49/20	6	−15/2	20/3	−15/4	6/5	−1/6		

Forward finite difference

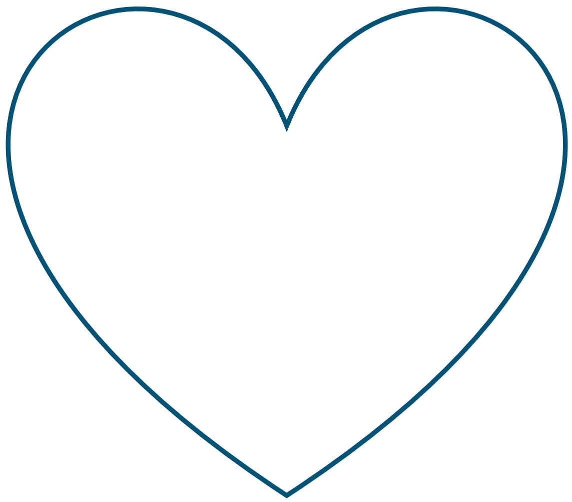
Derivative	Accuracy	−8	−7	−6	−5	−4	−3	−2	−1	0
1	1								−1	1
	2							1/2	−2	3/2
	3						−1/3	3/2	−3	11/6

Backward finite difference

Introducing a Mesh over Heart Domain, Ω

Geometry is:

- Complex
- Curved
- Sharp



Re-introducing a [Finite Difference] Mesh over Heart Domain, Ω

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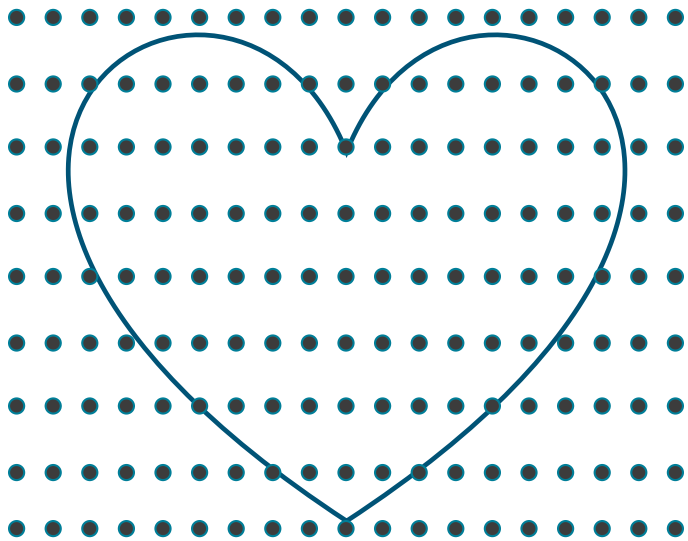

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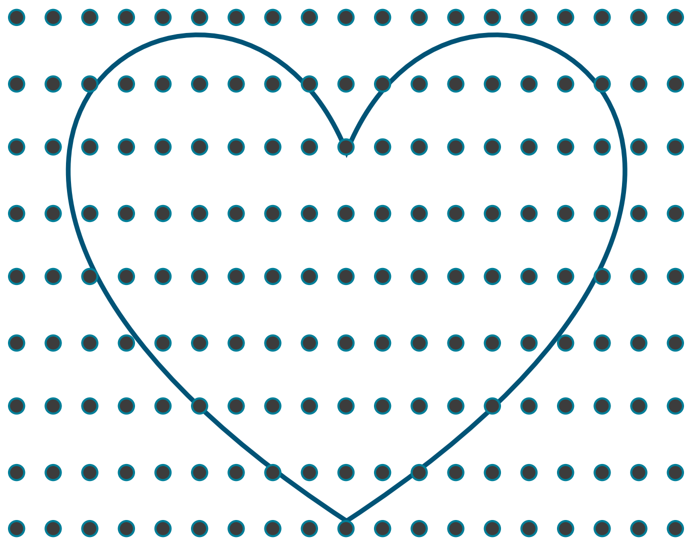
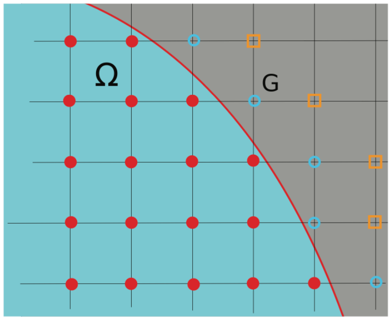


Not impossible: Chertock, et al., "A Second-Order Finite-Difference Method for Compressible Fluids in Domains with Moving Boundaries", Commun. Comput. Phys., 2018



Introducing a [Structured Mesh] over Heart Domain, Ω;

Geometry is:

- Complex
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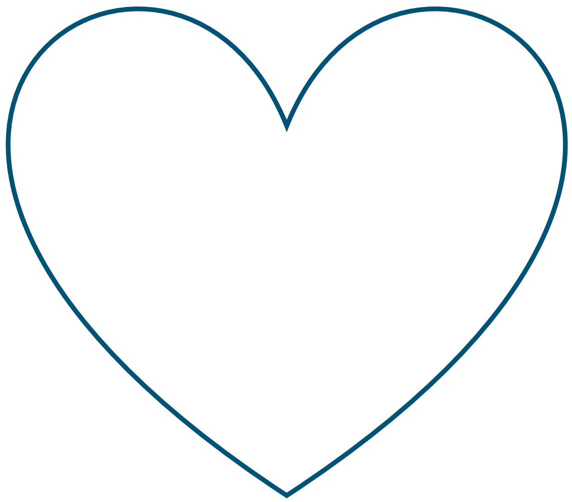

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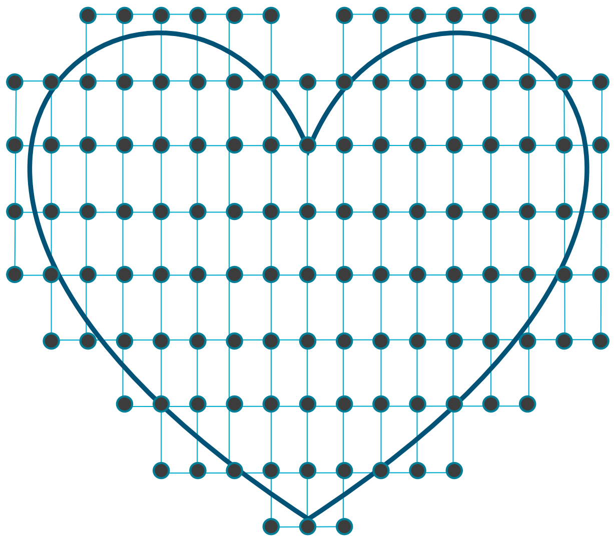

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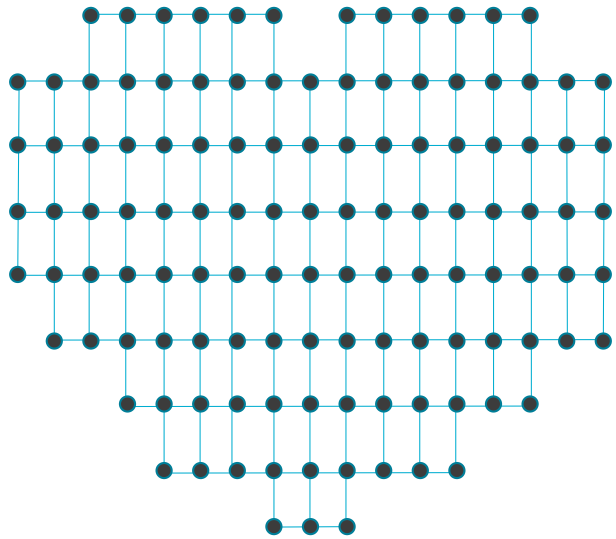
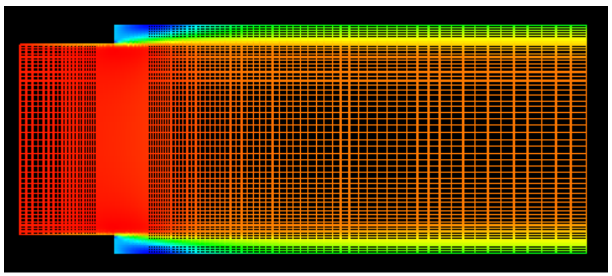
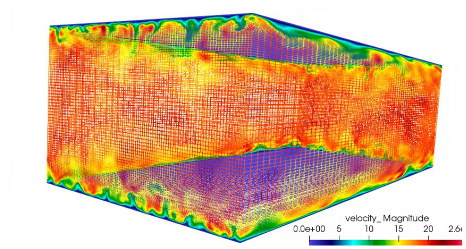


Structured vs Unstructured

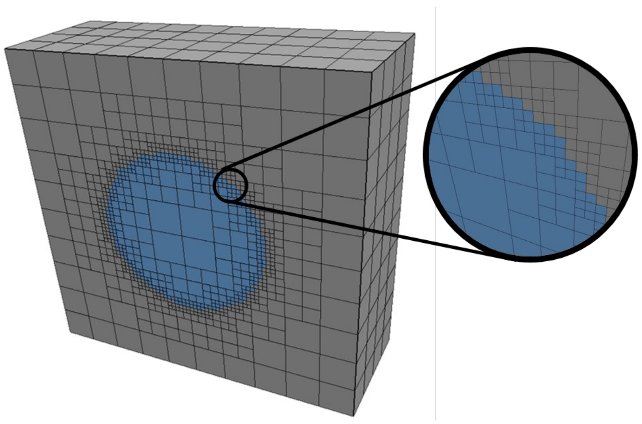
- Many times, canonical flows of interest are represented by simplified geometries that allow for cartesian meshes – with “stair-stepping”



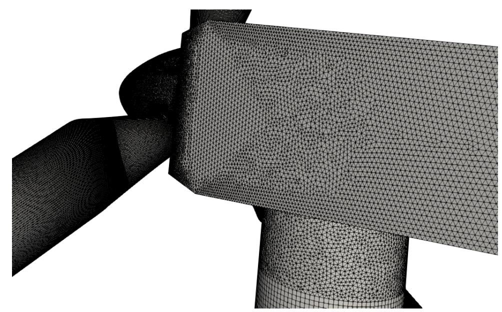
RANS-based backward facing step (Domino, 2012)



Re_τ 395 plane-channel (Jofre, Domino, Iaccarino, 2018)

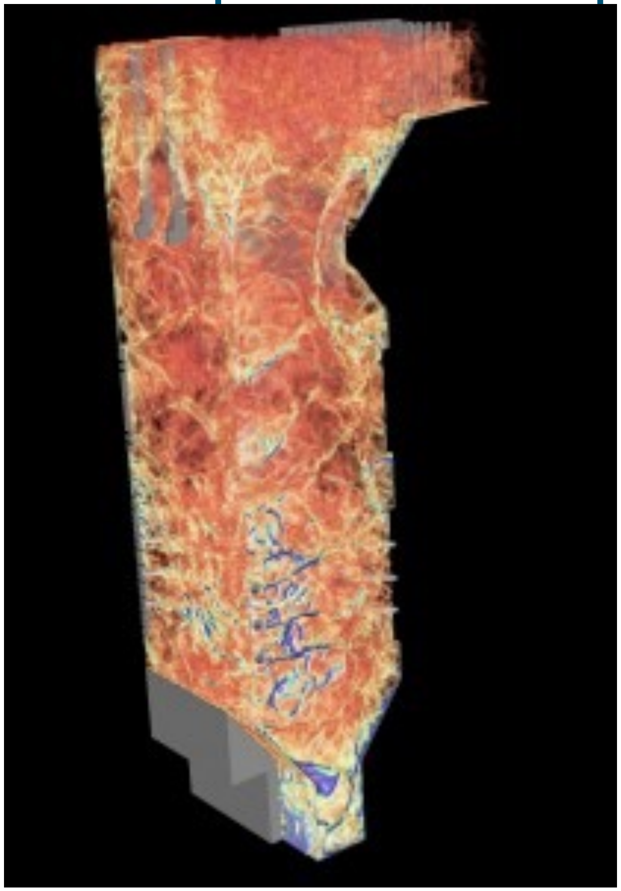


https://www.itascainternational.com/software/introduction-to-meshing



Often times, not!

Example:
The Carbon-Capture Multidisciplinary Simulation Center



http://ccmsc.utah.edu/about.html

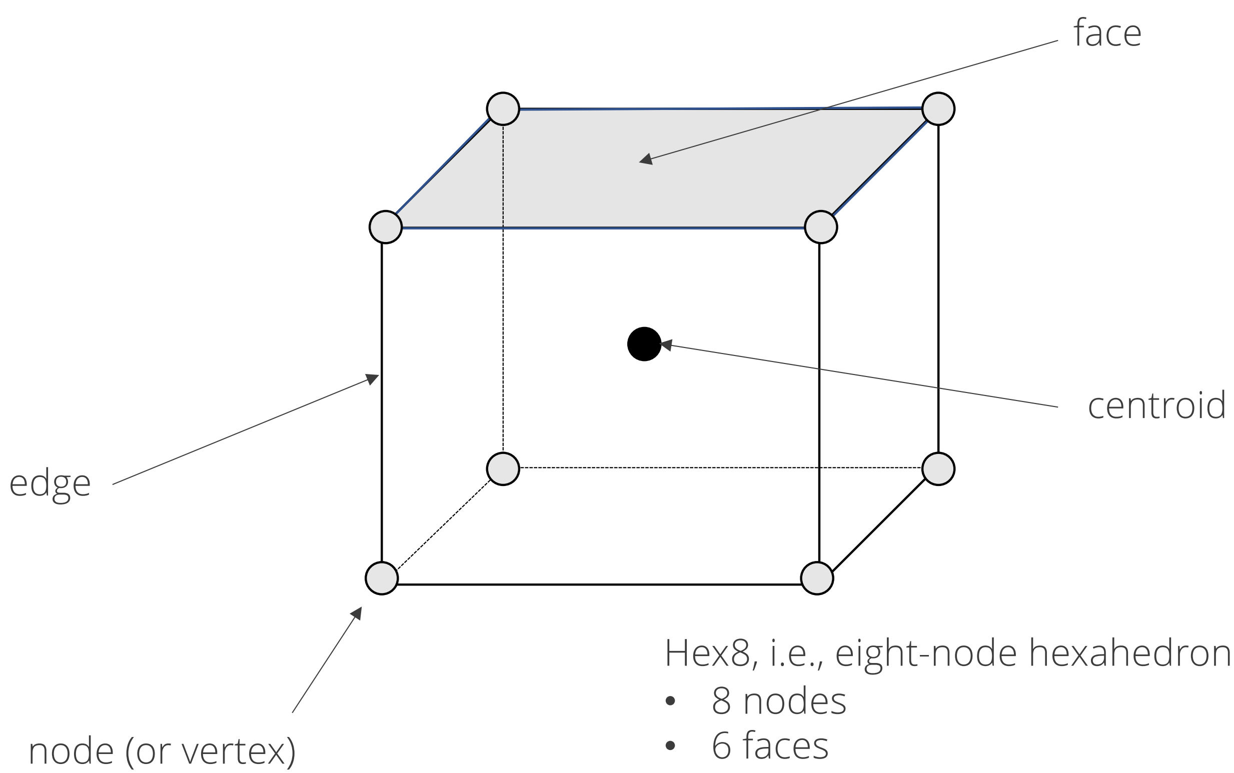
15MW coal-fired boiler volume rendered image of large (90 μm) particles

Staggered schemes have been demonstrated to support complex applications

Cut-cells and embedded approaches help

Attributes of an Element

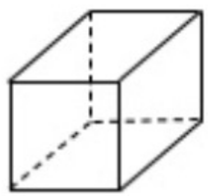
An element consists of nodes, edges, and faces

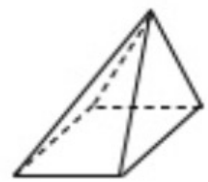
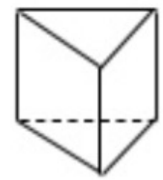


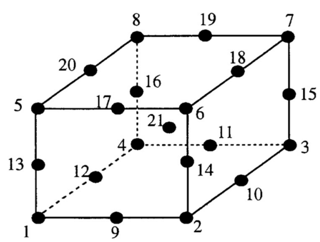
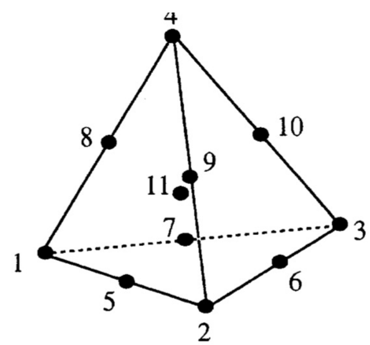
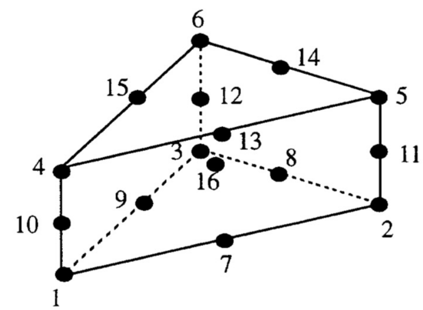
Hex8, i.e., eight-node hexahedron
- 8 nodes
- 6 faces
- 12 edges

Examples of Various Topologies

Hex8 Tet4 Pyramid5 Wedge6 Arbitrary



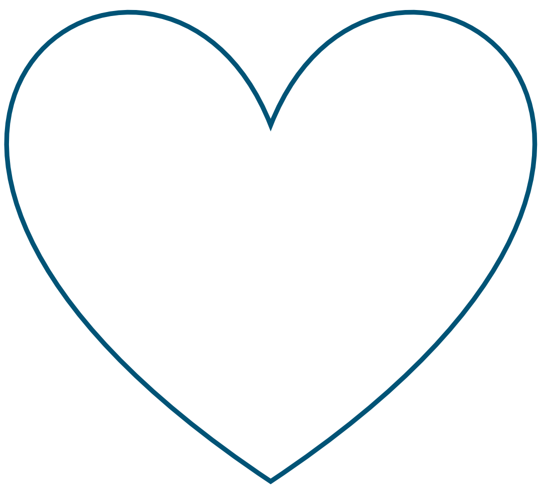



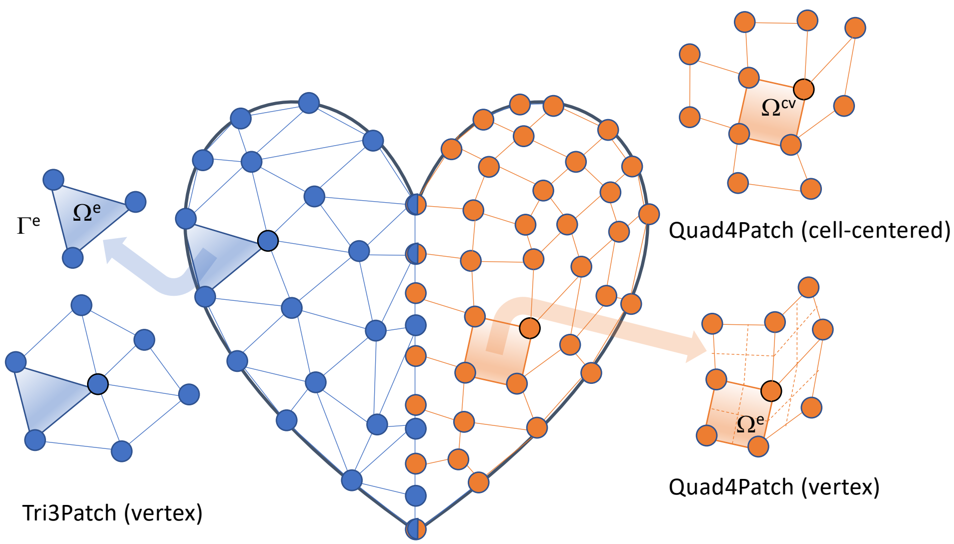





Higher-order promoted elements (Hex27, Tet10, Wedge16, Hex64, etc.)

Introducing a Mesh over Heart Domain, Ω

- Elements of size 4 (Quad4) or 3 (Tri3) have been introduced
- Exterior domain is faceted
- Non-conformal interface between the Tri3 and Quad4 block
- Two types of connectivity have been presented: node:element and element:face:element
- Two types of integration: Ω^e vs Ω^{cv}





Integration Over the Domain:
The "Finite" in Finite-Volume and Finite Element

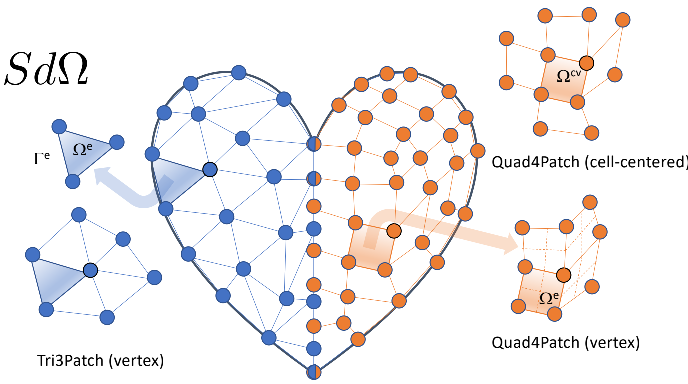
- Consider a simple model equation with the heart domain in mind:

$$\frac{\partial F_j}{\partial x_j} = S$$

Where F_j is a flux and S is a source term

- Integrating over the entire domain, Ω:

$$\int_{\Omega} \frac{\partial F_j}{\partial x_j} d\Omega = \int_{\Omega} S d\Omega$$



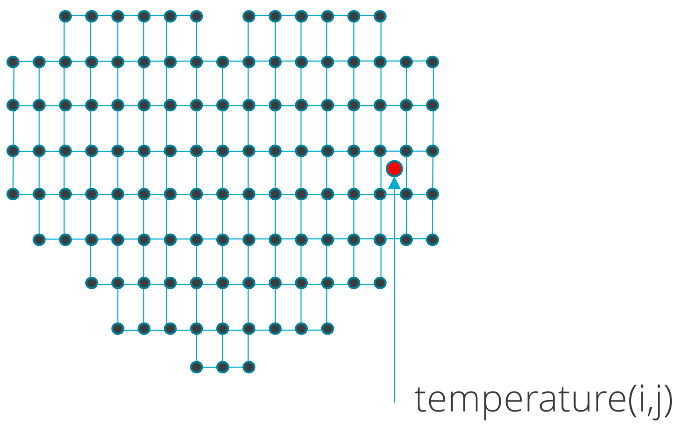
- Without loss of generality, let us define a set of subdomains, Ω_k:

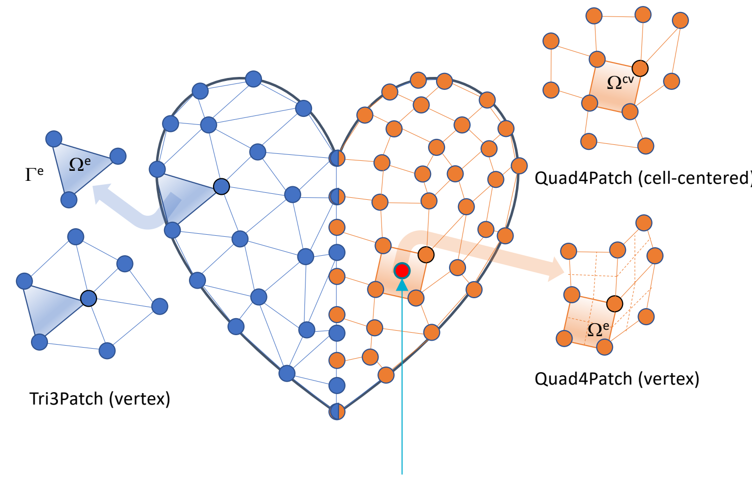
$$\sum_k \int_{\Omega_k} \frac{\partial F_j}{\partial x_j} d\Omega_k = \sum_k \int_{\Omega_k} S d\Omega_k$$

- As present, only volumetric integrals appear

Note:
- The formality of Σ_k and Ω_k is implied to exist over the full domain and is often times dropped – integral type implied by dV (volume) and dS (domain boundary)

Data Structure Ramifications: A bit more complex…





- Element and associated data structures are indexed directly via **i**$^{\mathbf{th}}$ and **j**$^{\mathbf{th}}$ location, e.g., **temperature** (i,j), over the range**: temperature**(0:nX-1,0:nY-1)
- Neighbors are directly indexed, e.g,, "north" neighbor of (i,j) is (i,j+1)

- Element and associated data structures are indexed indirectly via a data structure, e.g., **temperature(k)**, over the range: **temperature(0:nElem-1)**
- Nodes of element(k) are obtained via connectivity relationship mappings
  - **std::vector<mesh_type> nodes = elem_nodes (k)**
- Nodal fields, for element k via:
  - **pressure = field_data(nodes[0,..,numElem)**

Fundamentals of Discretization: Surface vs Volume Integrations

- Given a partial differential equation (PDE) and associated volumetric form:

$$\int \frac{\partial F_j}{\partial x_j} dV = \int S dV$$

- Applying Gauss Divergence provides the standard finite volume form for fluxes in surface integral form (no distinction between internal control volume faces and boundary faces):

$$\sum_k \int_{\Omega_k} \frac{\partial F_j}{\partial x_j} d\Omega_k = \sum_k \int_{\Omega_k} S d\Omega_k \longrightarrow \sum_k \int_{\Gamma_k} F_j n_j d\Gamma_k = \sum_k \int_{\Omega_k} S d\Omega \longrightarrow \int F_j n_j dS = \int S dV$$

- We can also multiple PDE by an arbitrary test function, w, and integrate over a volume,

$$\int w \frac{\partial F_j}{\partial x_j} dV = \int w S dV$$

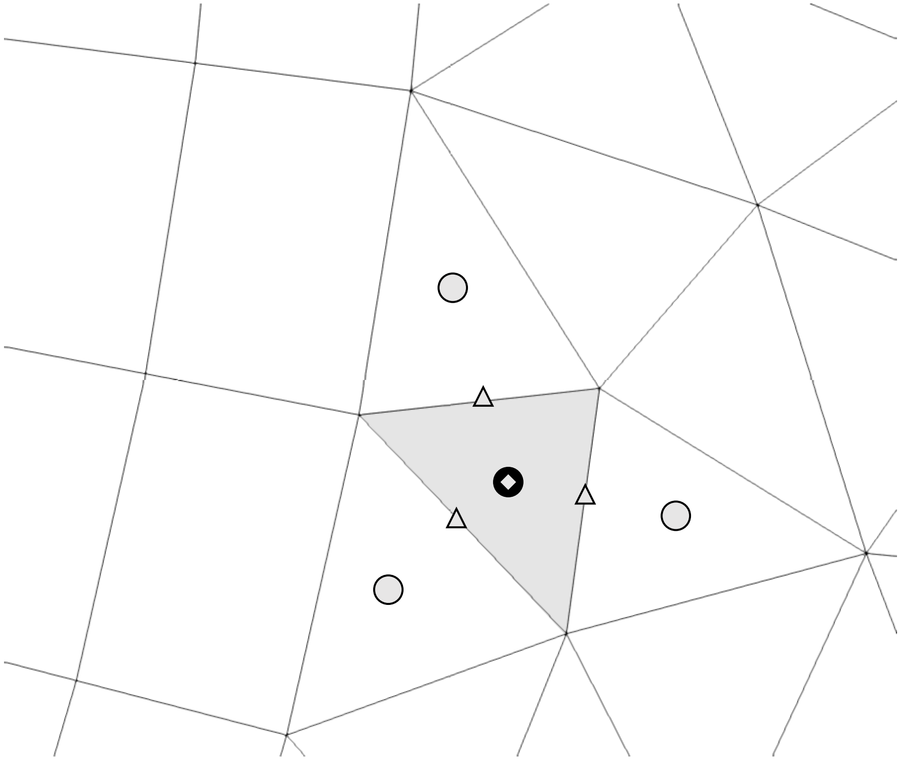
Next, integrate by parts and apply Gauss-Divergence. Note, that test function must be differentiable – shown here, at least once..

$$-\int F_j \frac{\partial w}{\partial x_j} dV + \int \frac{\partial w F_j}{\partial x_j} dV = -\underbrace{\int F_j \frac{\partial w}{\partial x_j} dV}_{\text{Interior}} + \underbrace{\int w F_j n_j dS}_{\text{Boundary}}$$

$$\frac{\partial w F_j}{\partial x_j} = w \frac{\partial F_j}{\partial x_j} + \frac{\partial w}{\partial x_j} F_j$$

Define a Stencil: Element:Face:Element

- Cell-centered, finite volume (shaded region)
  - Degree of freedom (DOF), i.e., solution, resides at the centroid of the element



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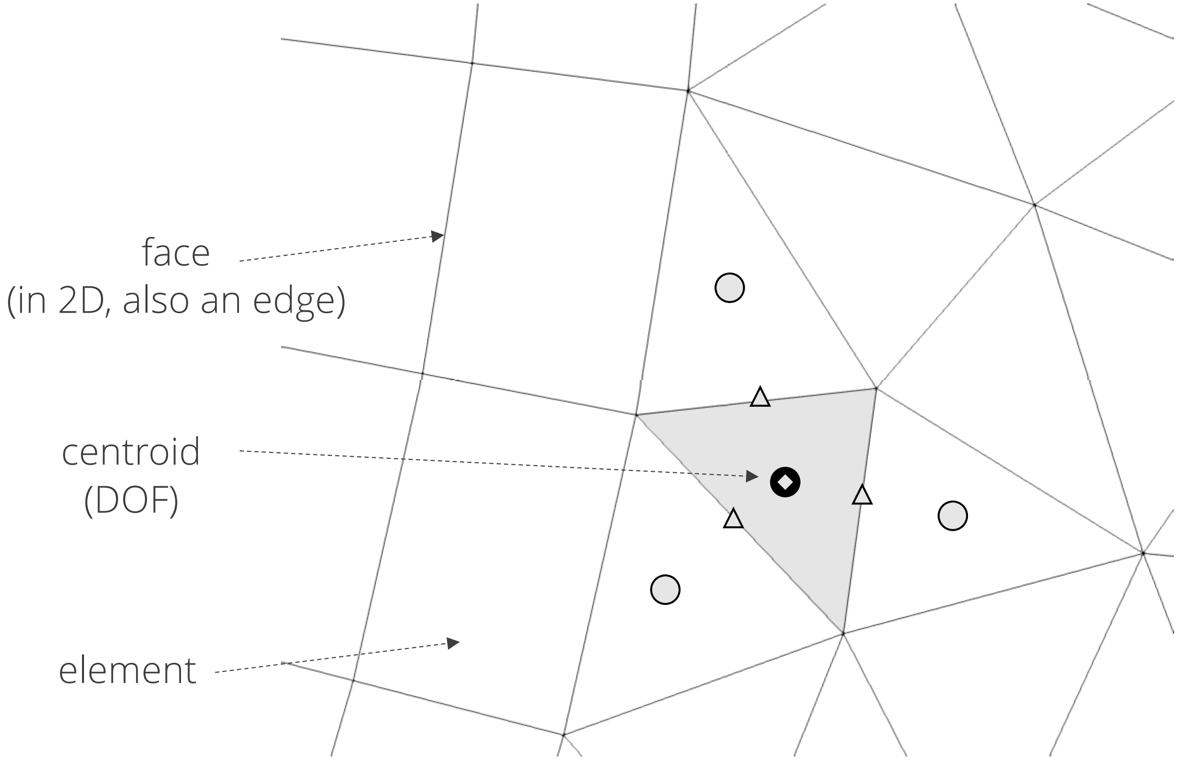

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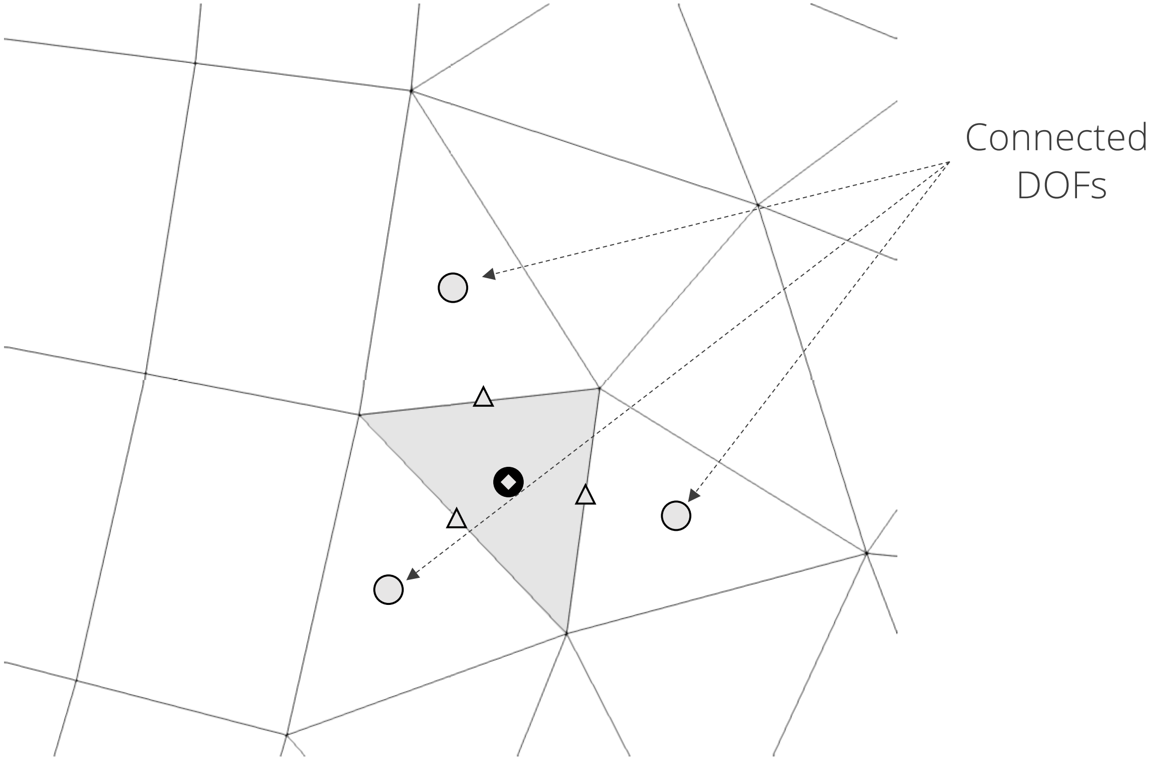

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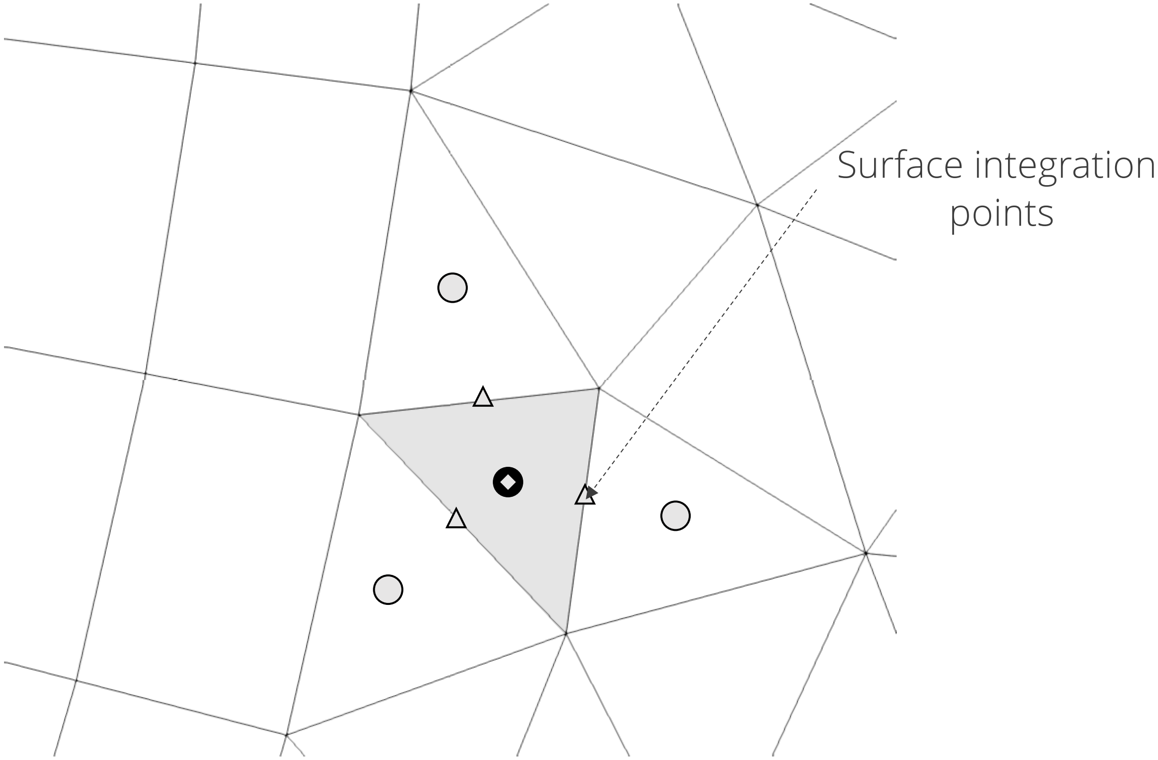

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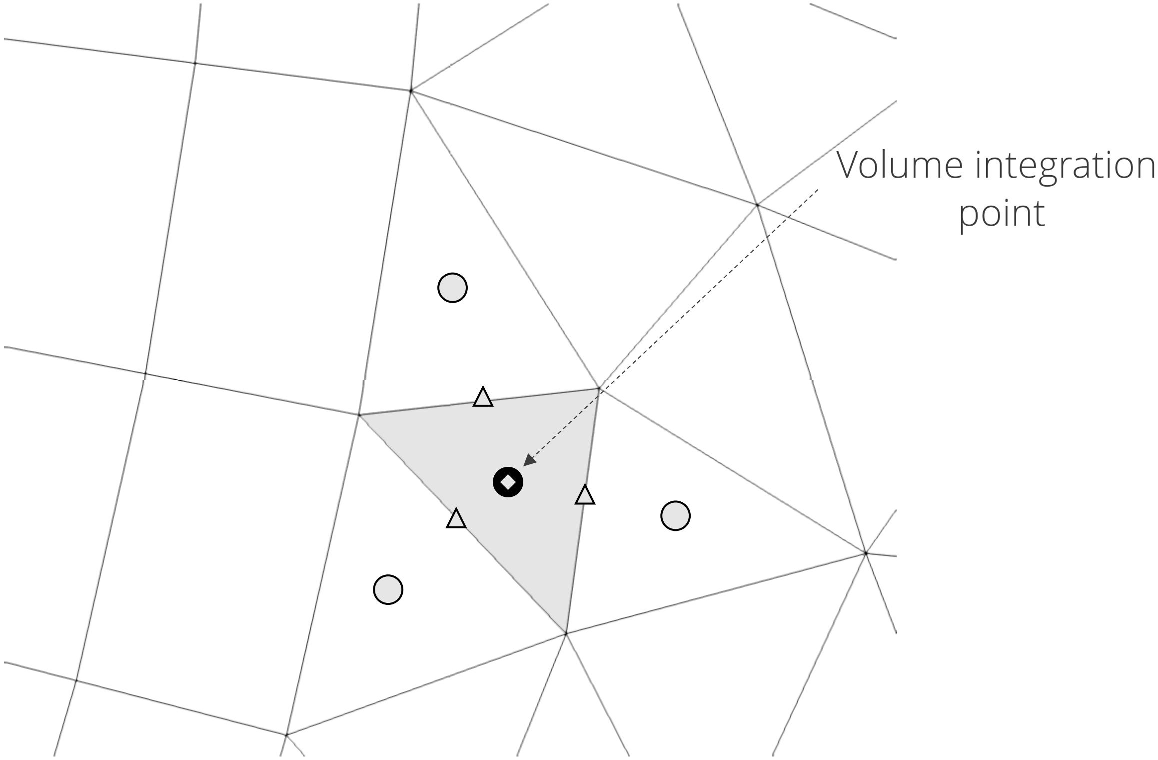
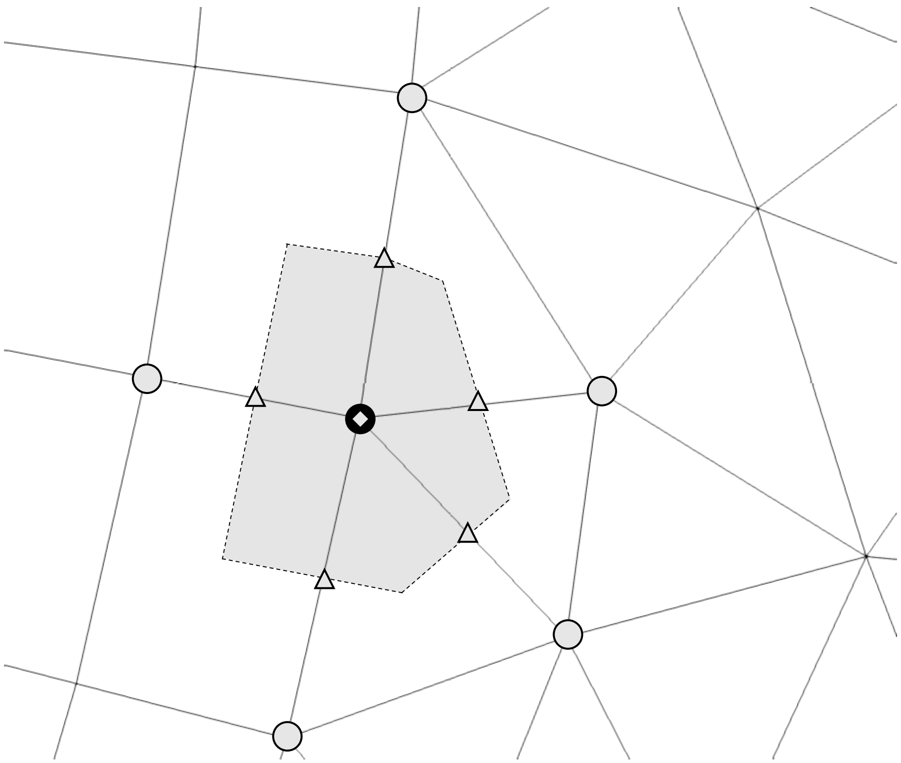


Define a Stencil: Node:Edge:Node

- Edge-based, vertex (or node)-centered finite volume (shaded region)
  - Degree of freedom, i.e., solution, resides at the node, or vertex



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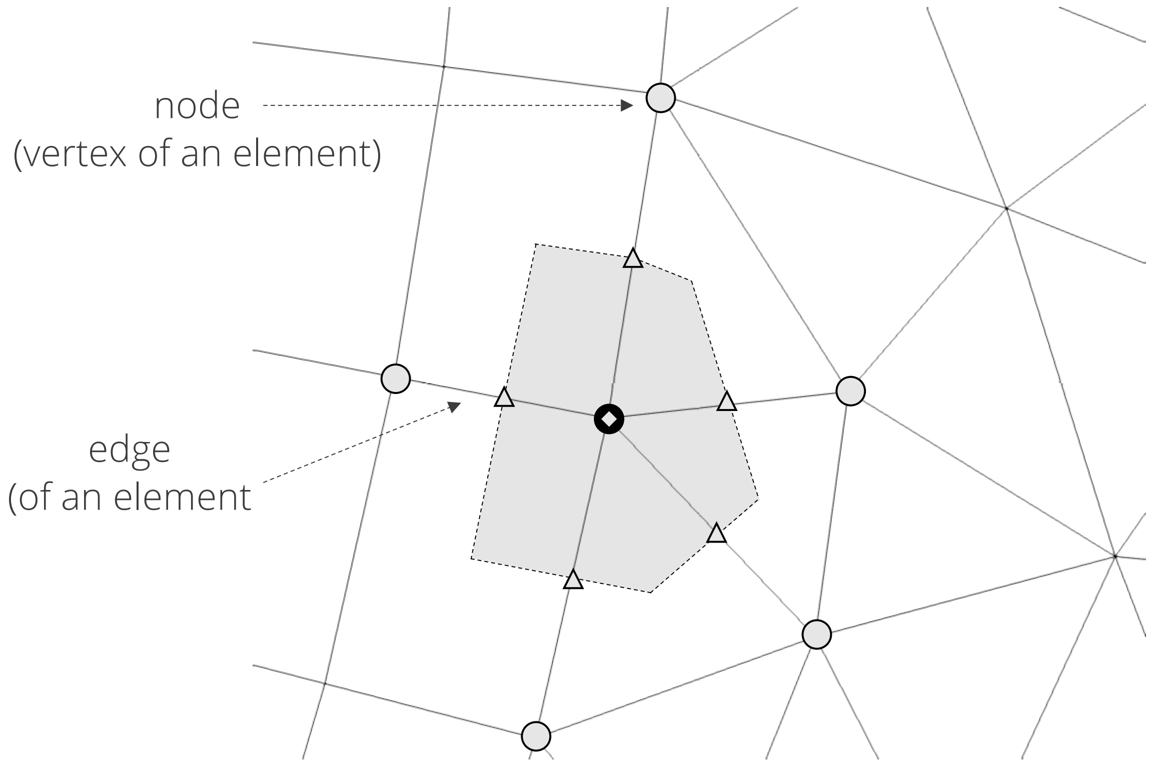

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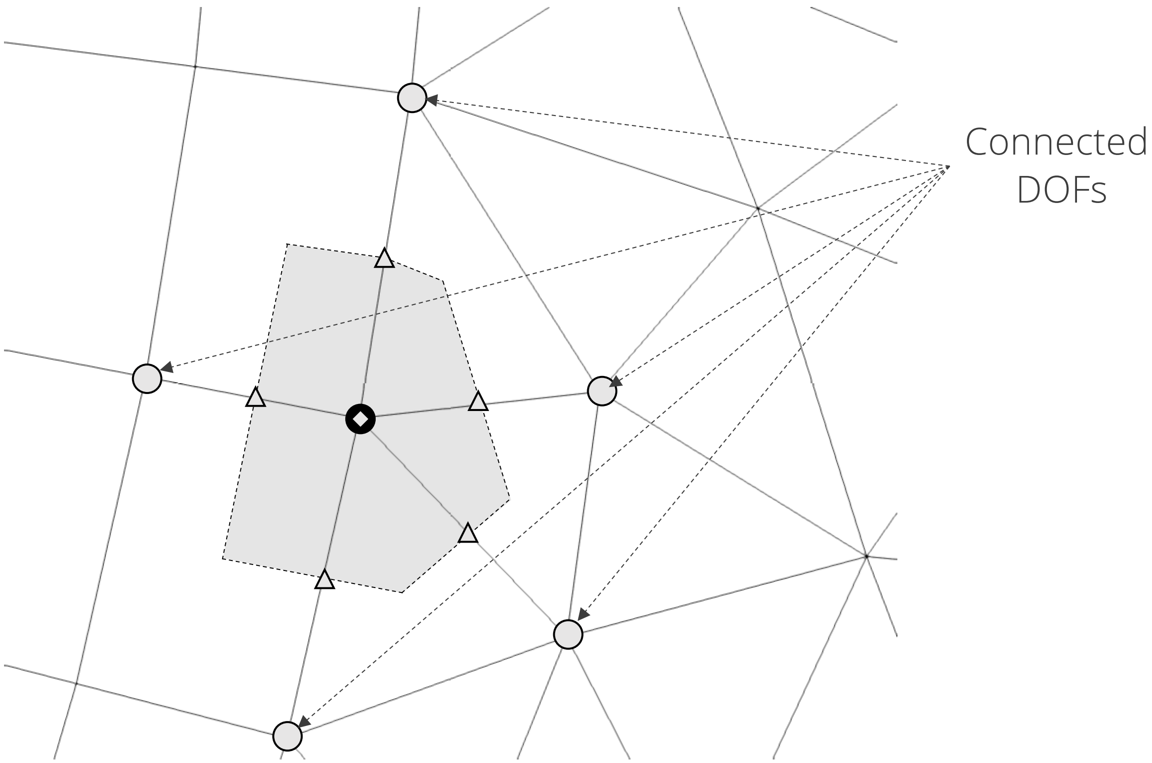

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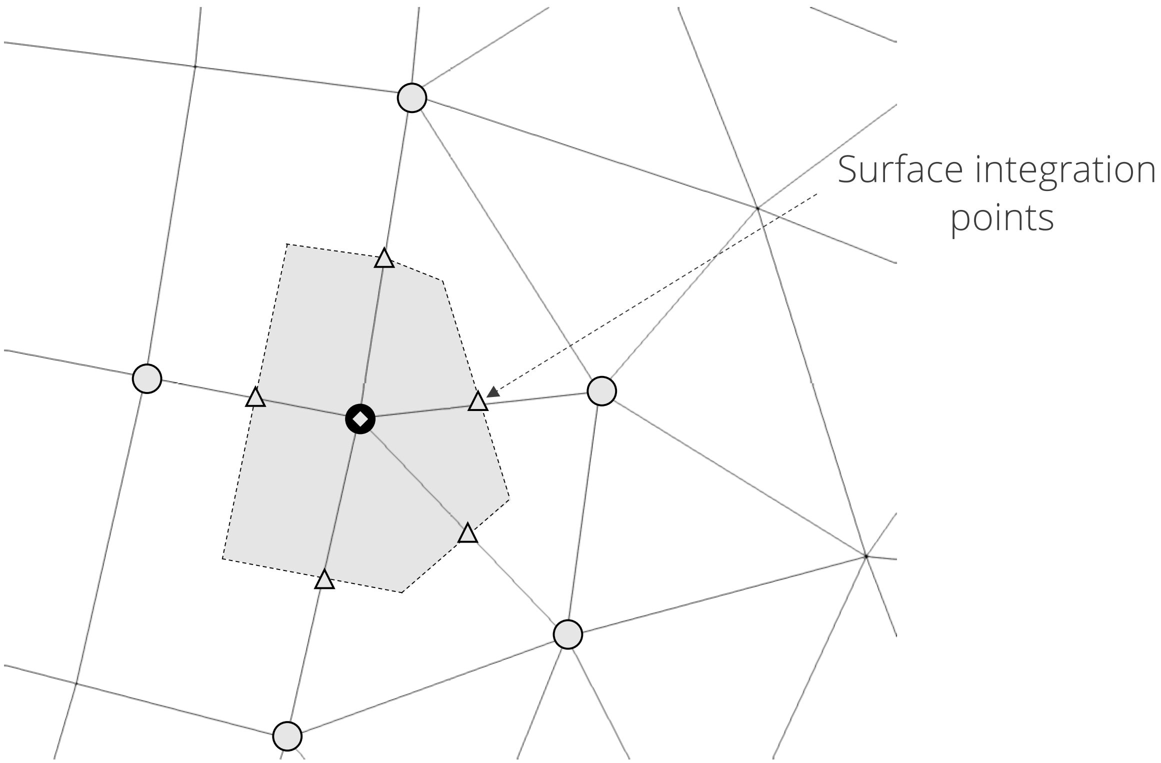

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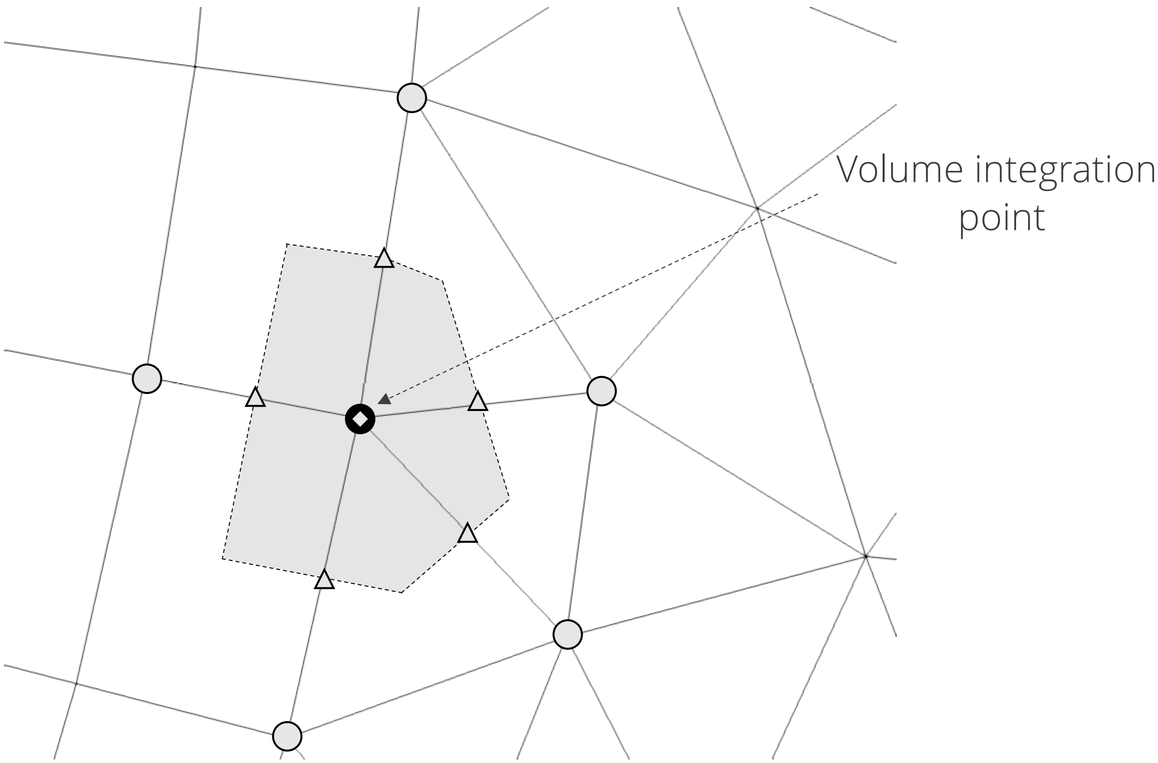
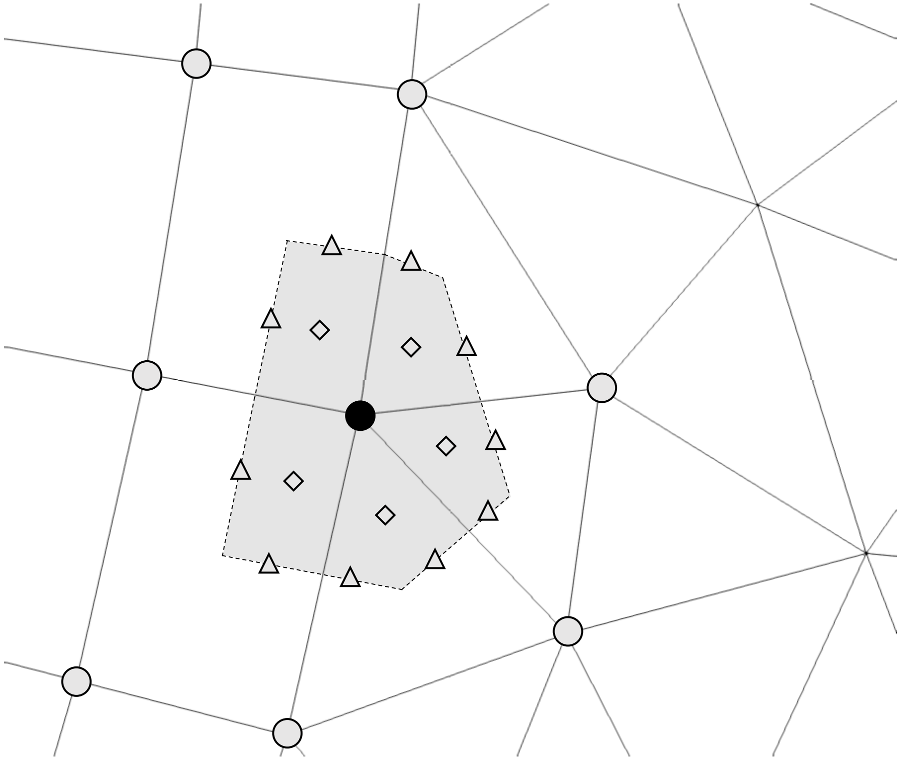


Define a Stencil: Node:Element:Node

- Choice #1, Element-based, vertex (or node)-centered finite volume (shaded region)
  - Degree of freedom, i.e., solution, resides at the node, or vertex



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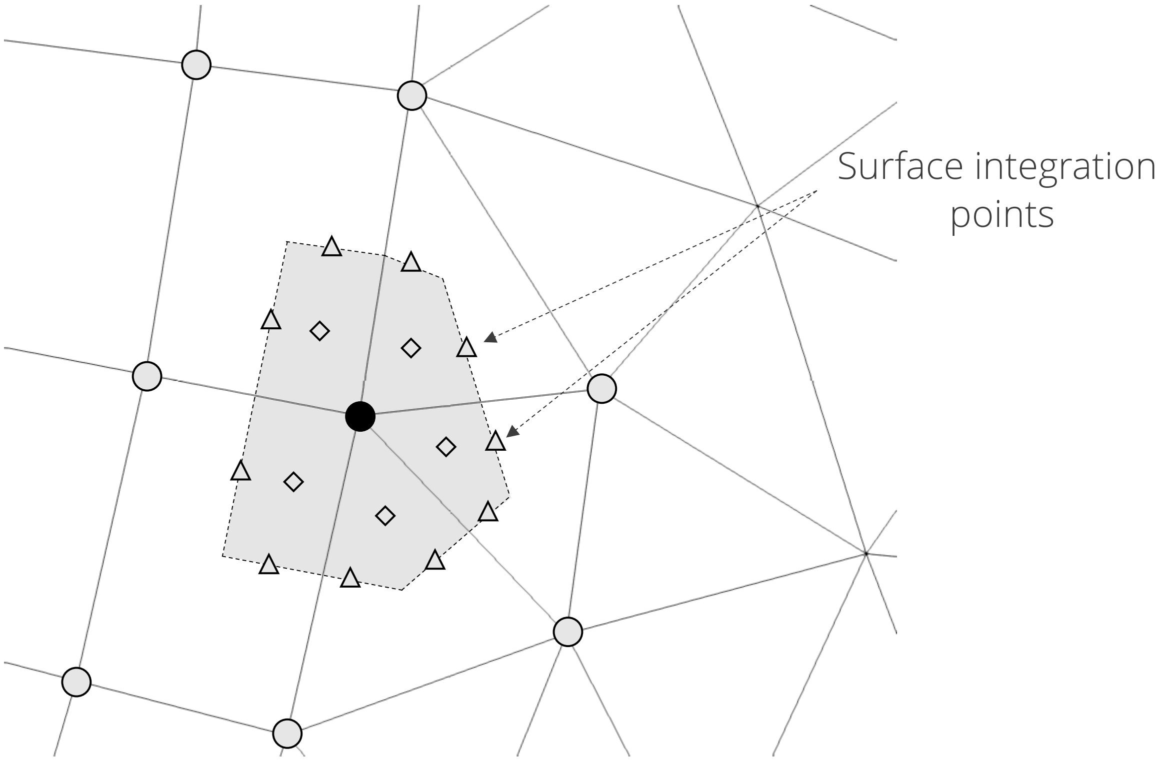

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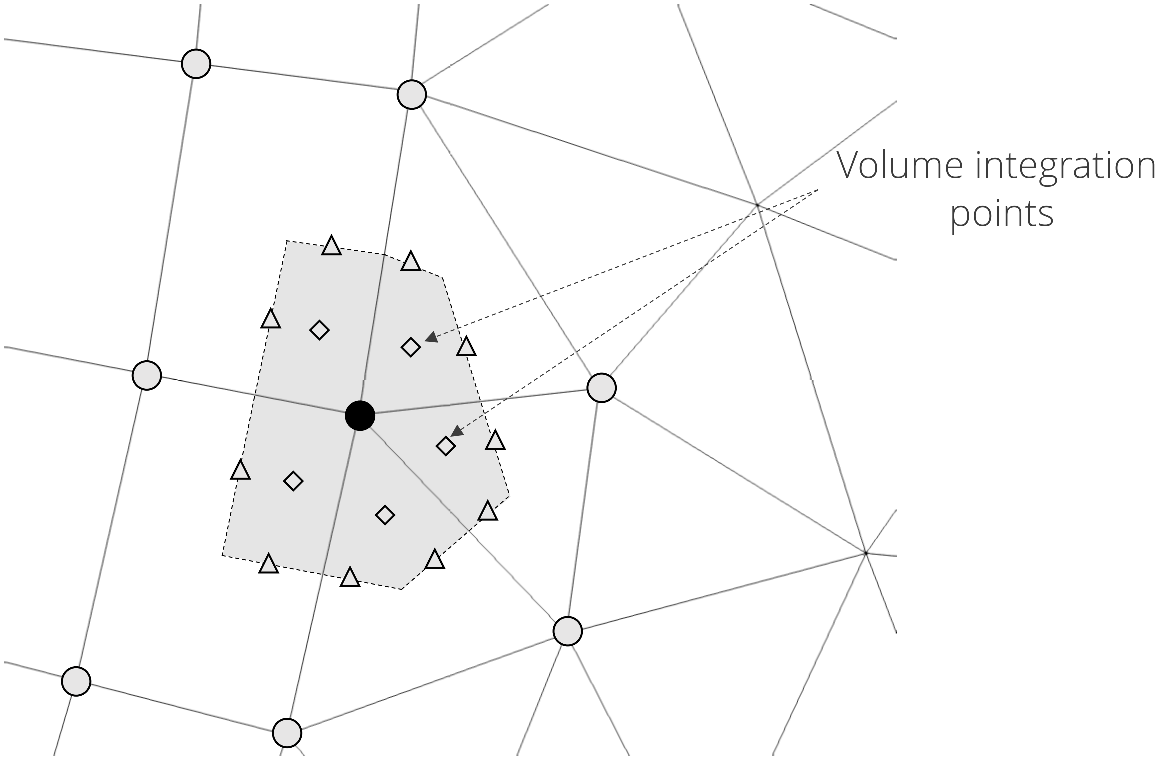
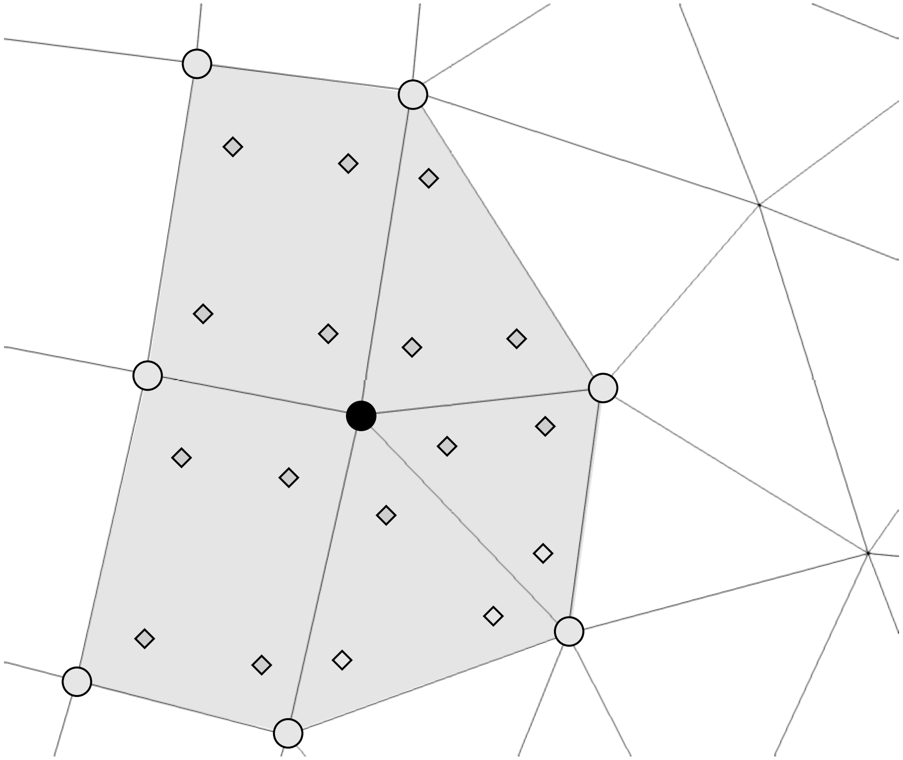


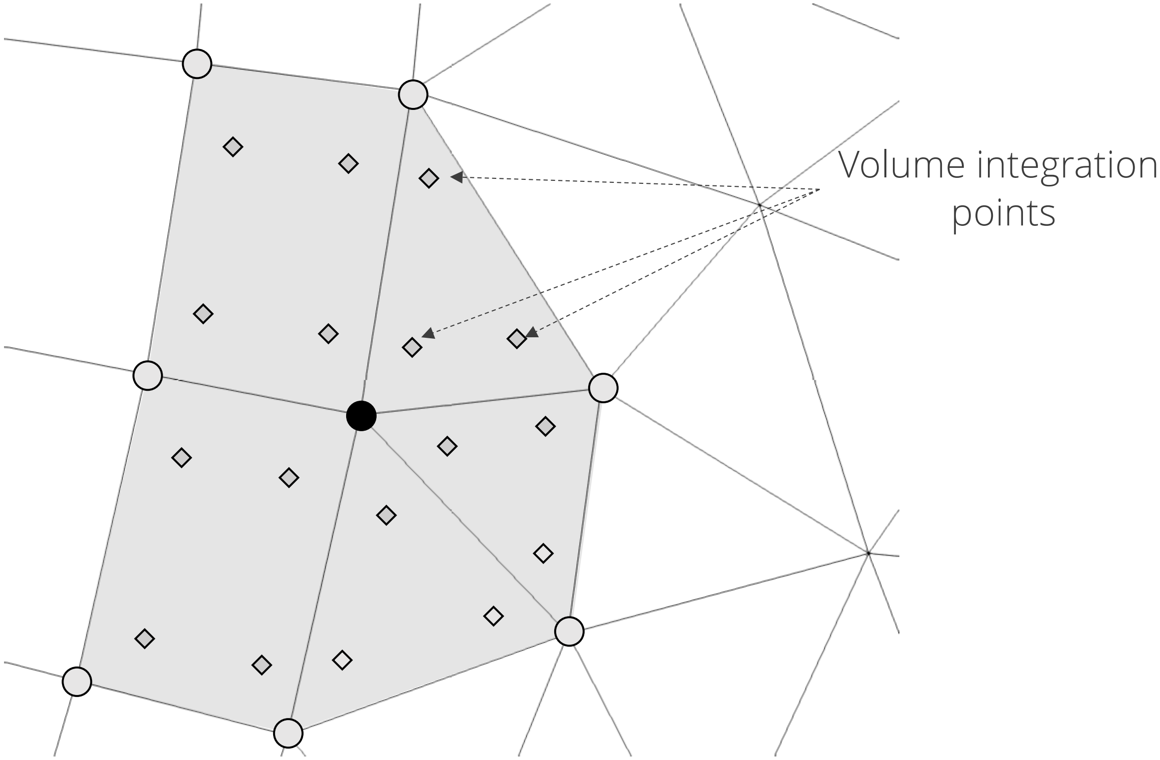
Define a Stencil: Node:Element:Node

- Choice #2, Element-based, finite element
  - Degree of freedom, i.e., solution, resides at the node, or vertex



Define a Stencil: Node:Element:Node

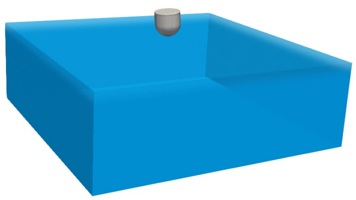
- Choice #2, Element-based, finite element
  - Degree of freedom, i.e., solution, resides at the node, or vertex



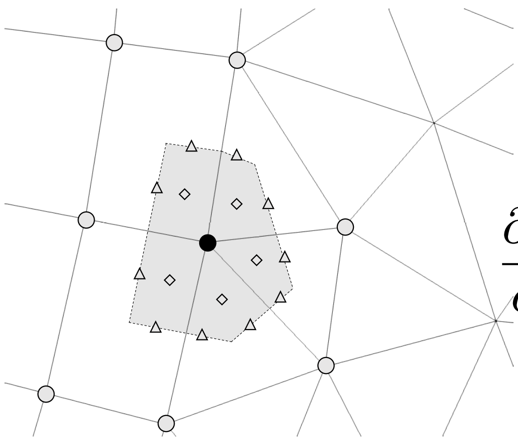
VOF Transport Discretization Nuance: Volume- or Surface-based?

- Simple enough, define the volume (fraction) of fluid (absent evaporation): $\frac{\partial \alpha}{\partial t} + u_j \frac{\partial \alpha}{\partial x_j} = 0$

Option 1: volumetric-form: $\int \frac{\partial \alpha}{\partial t} dV + \int u_j \frac{\partial \alpha}{\partial x_j} dV = 0$



CVFEM/FEM (really, any element-based approach)
Evaluated as a volumetric-contribution (diamonds)



$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$

$$\frac{\partial \phi_{ip}}{\partial x_j} = \sum_n \frac{\partial N_n^{ip}}{\partial x_j} \phi_n$$

Option 2: divergence-form:

$$\int \frac{\partial \alpha}{\partial t} dV + \int \frac{\partial \alpha u_j}{\partial x_j} dV - \int \alpha \frac{\partial u_j}{\partial x_j} dV = 0$$

Gauss-Divergence $\int \alpha u_j n_j dS$

Traditional finite volume (element, edge, cell-centered)
Evaluated as a surface integral (triangle)

Allows for a consistent advecting velocity (mass conserving) that is obtained from the continuity equation

Linking to **1d_quad4_adv_diff**

Recall, the transport equation for the 1d_quad4_adv_diff laboratory exercise is as follows:

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} + \frac{\partial q_j}{\partial x_j} = 0 \quad \text{where} \quad q_j = -\nu \frac{\partial \phi}{\partial x_j}$$

For now, let's focus on the advection term. We know that we can integrate over the volume and simply compute this term at the volume integration points,

$$\int u_j \frac{\partial \phi}{\partial x_j} dV$$

Option: **scv_advection_np**

As with the volume of fluid equation on the previous slide, we can also write this term as:

$$\int u_j \frac{\partial \phi}{\partial x_j} dV = \int \frac{\partial u_j \phi}{\partial x_j} dV - \int \phi \frac{\partial u_j}{\partial x_j} dV$$

that can be simplified (for constant velocity)

$$\int u_j \frac{\partial \phi}{\partial x_j} dV = \int u_j \phi n_j dS$$

Option: **scs_advection_np** (or **scs_upw_advection_np**)

Linking to **1d_quad4_adv_diff**

Recall, the transport equation for the 1d_quad4_adv_diff laboratory exercise is as follows:

$$\frac{\partial \phi}{\partial t} + u_j \frac{\partial \phi}{\partial x_j} + \frac{\partial q_j}{\partial x_j} = 0 \quad \text{where} \quad q_j = -\nu \frac{\partial \phi}{\partial x_j}$$

For now, let's focus on the advection term. We know that we can integrate over the volume and simply compute this term at the volume integration points,

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Q: Is this really simple for all of the schemes we have discussed?

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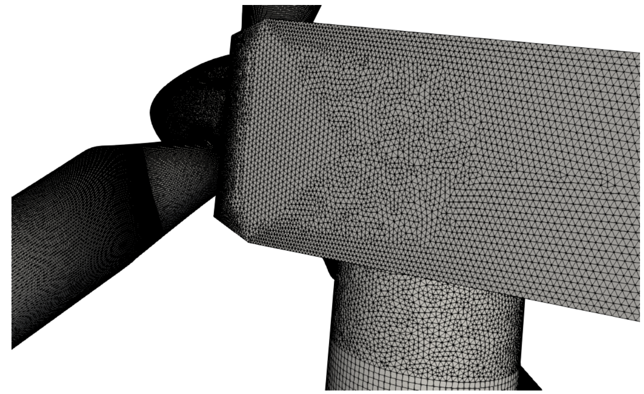
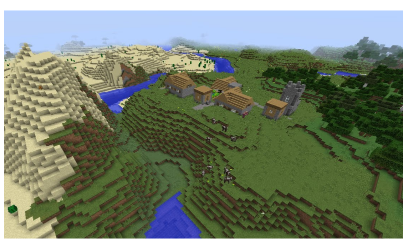
Reality: Meshing time for complex applications remains a significant bottleneck!

- Many applications of interest contain complex geometries low-Mach fluids users interested in high-quality simulation results tend towards hexahedral-based topologies (if possible)
- However, if a scheme is "design-order" accurate, any topology may suffice as it is simply a matter of mesh size and efficiency – not unlike the active discussion on low- vs higher-order
- Sometimes, the penetration of a low-Mach fluids physics addition in common analysis is high as the meshing can be prohibitively complex



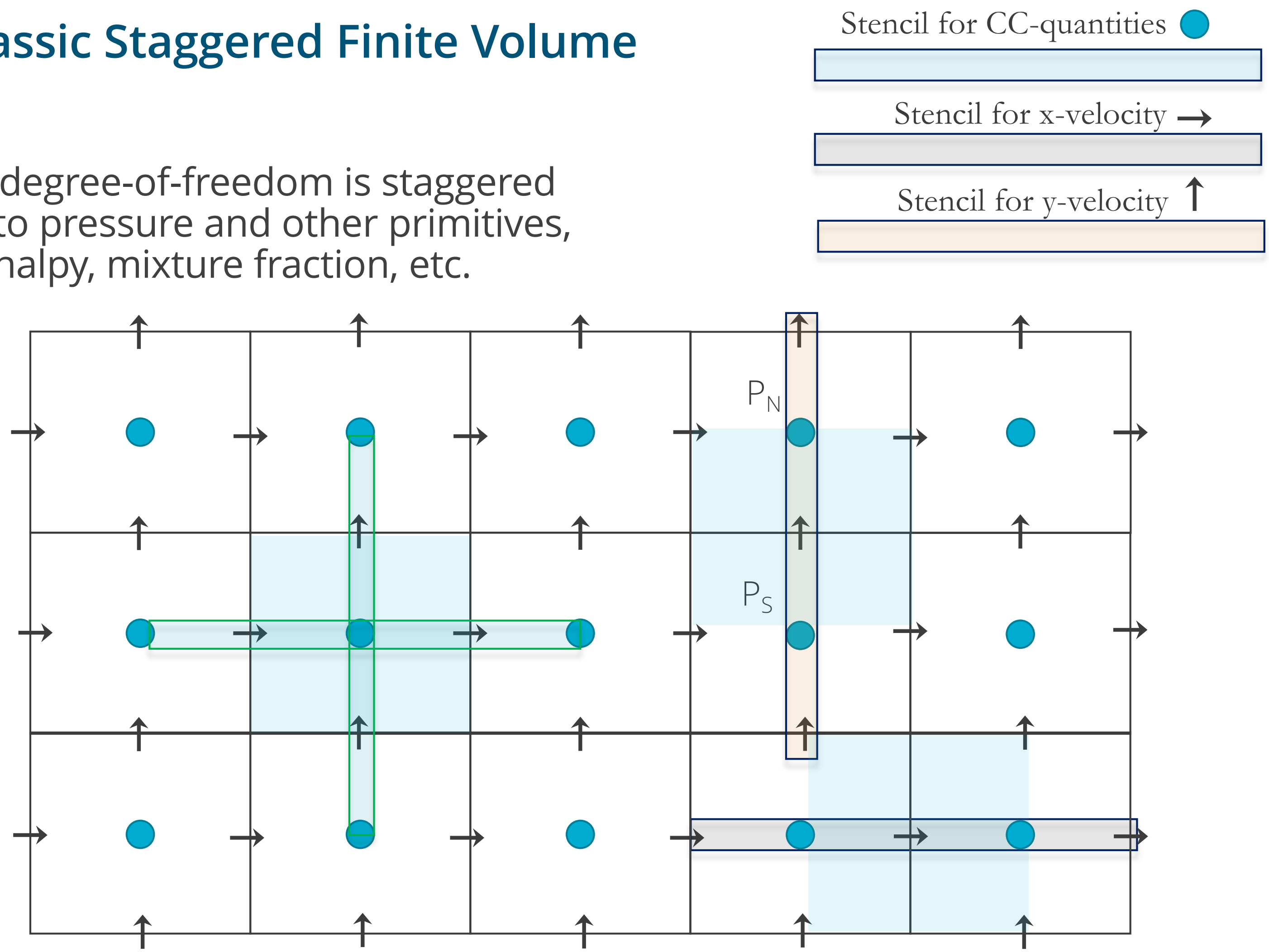
Example: Vestas V27 225 kw hybrid low-order Hex8/Tet4/Pyr5/Wedge6



Very complex world – stair-stepped!

Classic Staggered Finite Volume

- Velocity degree-of-freedom is staggered relative to pressure and other primitives, e.g., enthalpy, mixture fraction, etc.



Attributes of a Staggered Scheme

- By design, non-orthogonality is absent, however, complex geometry will be stair-stepped
- From a fluids perspective, the operators are ideal, i.e., pressure gradient for momentum is compact, e.g., $(P_E - P_W)\Delta x^{-1}$
- As will be seen in future lecture topics, the skew-adjoint nature of the Divergence operator, **D**, and Gradient operator, **G**, allows for a Laplace operator, **L** = **DG**
- Can be extended to higher-order
- Frequently, meshing complex geometries can be extremely difficult (consider our V27 example)

An Informal Survey….

- Cell-Centered: (Sometimes generalized Polyhedra)
  - Ansys Fluent, OpenFOAM (FireFOAM, NavyFOAM), CD-Adapco (Star-CCM), Soleil-X (Stanford)
- EBVC: (Most typical in the acoustically compressible space)
  - SU2, FUN3D, CHAD, Nalu-Wind (production), Nalu (option to explore discretizations)
- CVFEM
  - Fluent (originally!), CFX-TASC-FLOW, Sierra Fuego (SNL), Nalu
- FEM
  - FIDAP, COMSOL, EDDY (NASA), AcuSim, PHASTA
- Staggered
  - Arches (Utah)

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Common Water-Cooler CFD Arguments:

- Structured vs. Un-structured
- FEM vs. Finite Volume
- Node-centered vs. Cell-centered
- Monolithic vs. Operator Split
- Compressible vs. (acoustically) Incompressible
- Explicit vs. Implicit

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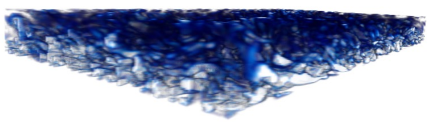
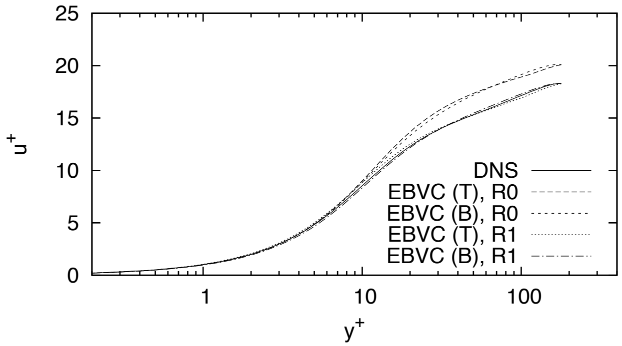
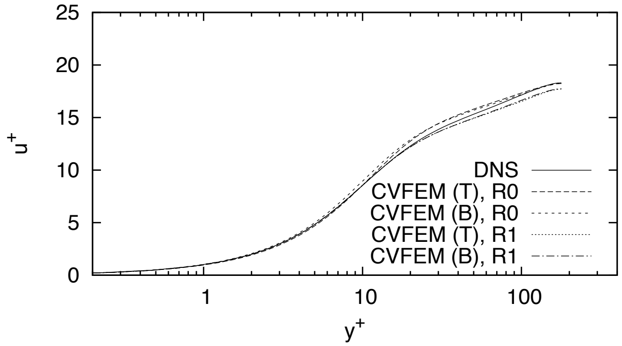
NALU LOW-MACH

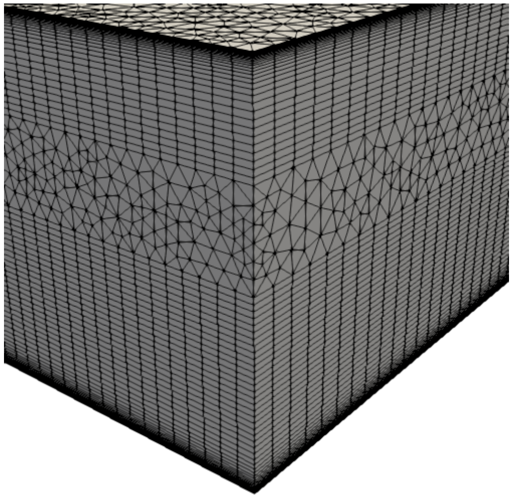
Hybrid Meshes, Even for LES!



- Hybrid mesh study based on Ham and Iaccarino, *CTR Annual Brief*, 2006, found that simulations were extremely sensitive to mesh topology
- Non-symmetric time mean flow found for cell-centered; better for the CTR node-centered formulation
- Native CVFEM and EBVC are both symmetric in mean quantities







Domino, et. al, "The suitability of hybrid meshes for low-Mach large-eddy simulation" Stanford CTR Summer Program, 2018

Recent Generalized Unstructured Findings

- Domino, et. al, "*An assessment of atypical mesh topologies for low-Mach large-eddy simulation*", Comput. Fluids (2019)